Explosive Equation-of-State Code

Reassessing LLNL's predictive capability for explosive performance

Unfortunately, no capability exists in high explosives that allows performance predictions on unknown systems. Past data, ordinarily a valuable source of predictive material, is seldom available.

At LLNL, we recently assembled decades of cylinder-test and plate data into the report *Detonation Equation of State at LLNL, 1993*. The information in this document covers homogeneous and some heterogeneous explosives; the vast area of composite explosives has yet to be explored.

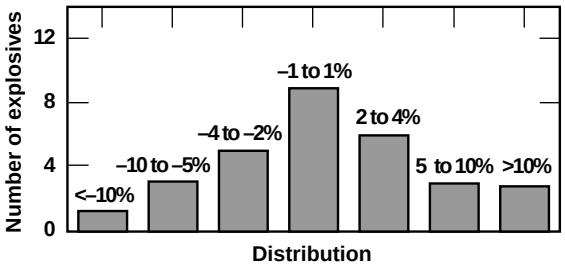
CHEETAH and the future

The only available predictive capability lies in thermochemical modeling, which takes density, heat of formation, and composition and calculates the explosive adiabat and the total energy of detonation. We have surpassed the old American standard, TIGER, with the new code, CHEETAH. The new code is more robust; faster; user friendly with respect to input, output, and operation; and fits to the JWL equation-of-state function. This new code points up the need for an improved thermodynamic library for liquid and solid products.

The first version of CHEETAH has both the BKW-R (gas model with compressibility) and JCZ3 (intermolecular potential model) equation-of-state models normalized to detonation velocities (similar to the TIGER code). The first version was available in the summer of 1994.

APPLICATIONS

- *Detonation code for composite formulations*
- *Explosive modeling for mining and petroleum exploration*
- *Modeling of propellants, combustion, and chemical reactivity (unnormalized)*
- *Extensions to low concentrations suitable for environmental evaluation of explosives*



CHEETAH can calculate energies on the adiabat. Here, we show the distribution of percent agreement of the BKW-R code with measured LLNL cylinder results for 30 homogeneous explosives. The relative volume used is 4:1, and the PETN correction has been made to the calculated energies.

A second version, available by summer 1995, incorporates new versions of BKW and JCZ, which are normalized to detonation velocities, detonation pressures, and energies on the adiabat derived from cylinder test data. In addition, the new version has a refitted solids library with compressibility and the ability to handle the various carbon phases.

Availability: We are interested in collaborating with academia or industry in the pooling of information on explosive performance and the predictive modeling of this data.

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